

On the Origin of the Tunneling Asymmetry in the Cuprate Superconductors: a variational perspective

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(Dated: February 6, 2008)

Through variational Monte Carlo calculation on Gutzwiller projected wave functions, we study the quasiparticle(qp) weight for adding and removing an electron from a high temperature superconductor. We find the qp weight is particle-hole symmetric at sufficiently low energy. We propose to use the tunneling asymmetry as a tool to study the mechanism of electron incoherence in high temperature superconductors.

PACS numbers:

The scanning tunneling microscopy (STM) plays an important role in the study of the high temperature superconductors since it can provide local information on the single particle properties with ultrahigh energy resolution. A striking feature in the STM spectrum of the high temperature superconductors is their remarkable particle-hole asymmetry. The hole side of the spectrum always dominates the particle side of the spectrum in hole doped cuprates[1].

This asymmetry is not at all surprising if we take the high temperature superconductors as a doped Mott insulators described by the $t - J$ model. In such a doped Mott insulator, an added electron has a reduced probability to contribute to the electron spectral weight in the low energy subspace of no doubly occupancy. More specifically, if the hole density in the system is x , then the total spectral weight in the particle side of the spectrum is reduced to x , while the total spectral weight in the hole side of the spectrum is not affected by the no double occupancy constraint. Thus the total spectral weight is particle-hole asymmetric for small x . However, such an asymmetry on the total spectral weight tells us nothing about the distribution of the spectral weight at low energy. To address the problem of tunneling asymmetry in the near vicinity of the chemical potential, we need more detailed information on the low energy excitation of the system.

Rantner and Wen addressed this problem in the slave-Boson mean field theory of the $t - J$ model[2]. In their theory, the tunneling asymmetry comes from the incoherent part of the electron spectrum. In the slave-Boson mean field theory, an electron is split into two parts, namely the Fermionic spinon part that carries spin and the Bosonic holon part that carries charge. The superconducting state is described by the Bose condensation of holons in the background of BCS pairing of spinons. In the presence of the holon condensate, the electron spectrum acquires a nonzero quasiparticle(qp) weight. In the mean field theory, the spectral weight in the particle side

of the spectrum is totally coherent since the holon removed during the particle injection process must originate from the holon condensate. However, the hole side of the spectrum involves both coherent and incoherent parts since the holon injected during the particle removing process can stay either in the condensate or out of it. In the slave-Boson mean field theory, the qp weight differs from the BCS result by a constant renormalization factor x , namely xu_k^2 for adding an electron and xv_k^2 for removing an electron. Thus if one neglects the asymmetry due to the band structure effect near the chemical potential, then the qp weight is particle-hole symmetric and tunneling asymmetry must originate from the incoherent part of the electron spectrum.

Recently, Anderson and Ong addressed the same problem with a variational approach[3]. They constructed the variational wave function for the ground state and the excited state of the $t - J$ model following the original RVB idea. In their treatment, the particle-hole asymmetry is taken into account explicitly in the variational wave function by the introduction of a fugacity factor $Z(= \frac{2x}{1+x})$. This fugacity factor is expected to play the role of the Gutzwiller projection into the subspace of no double occupancy. In this theory, the electron spectrum is dominated by the qp contribution and the tunneling asymmetry originates from the coherent rather than the incoherent part of the electron spectrum. Especially, when the excitation energy considered is much larger than the pairing gap (so that the particle-hole mixing due to the superconducting pairing is negligible), the qp weight for adding an electron is a factor Z smaller than that for removing an electron. In this theory, the qp weight for adding an electron scales linearly with the hole density x near half filling, while the qp weight for removing an electron scales linearly with $1 - x$. The problem of tunneling asymmetry and the qp weight is also addressed variationally in some other recent works[4, 5, 6, 7]. For example, it is proved by Yunoki that the electron spectral weight in the particle side is exhausted by the qp contribution

for a superconductor described by Gutzwiller projected BCS wave functions[5]. However, a clear understanding of the hole-like qp excitation of the Gutzwiller projected state is still absent.

In this paper, we show through the variational Monte Carlo calculation on Gutzwiller projected wave functions that the qp weight in the t-J model is particle-hole symmetric at sufficiently low energy. Especially, we find the qp weight for adding and removing an electron in a projected Fermi sea state both converge to the value determined from the jump of the momentum distribution function on the Fermi surface. We find the qp weight for adding and removing an electron both vanish at zero doping, as predicted by the slave-Boson mean field theory. However, the qp weight calculated from projected wave function show more complex momentum and doping dependence. We find the qp weight vanishes like x^{α_k} near half filling. The exponent x^{α_k} increases monotonically from $\frac{1}{2}$ to 1 when one move from deep inside the Fermi surface to far outside it in two spatial dimension. Thus the qp weight vanishes more slowly near zero doping than that predicted by the slave-Boson mean field theory. According to our result, the tunneling asymmetry near the Fermi level should be attributed to the incoherent part of the electron spectrum. We propose to use the tunneling asymmetry to study the mechanism of electron incoherence in the high temperature superconductors.

In the Landau theory of Fermi liquid, the quasiparticle plays a dual role. On the one hand, the qp can be thought of as a particle-like elementary excitation on the ground state of a N particle system. On the other hand, the qp can also be thought of as a constituent of the ground state of the $N + 1$ particle system, provided that the qp is located on the Fermi surface. The qp weight for adding an electron into the system on the Fermi surface is thus equal to the square of the matrix element of the electron creation operator between the ground state of N particle system and the ground state of $N + 1$ particle system,

$$Z_N^+ = |\langle g_{N+1} | c_k^\dagger | g_N \rangle|^2$$

while the qp weight for removing an electron from the system on the Fermi surface is equal to the square of the matrix element of electron annihilation operator between the ground state of N particle system and the ground state of $N - 1$ particle system,

$$Z_N^- = |\langle g_{N-1} | c_k | g_N \rangle|^2 = Z_{N-1}^+$$

In the thermodynamic limit, we have

$$Z_N^- = Z_{N-1}^+ \simeq Z_N^+$$

thus the qp weight should be particle-hole symmetric. This simple argument do not apply to the superconducting state. However, we do not expect the superconducting pairing to change the conclusion. The quasiparticle

in the superconducting state is a mixture of particle and hole components. Thus the superconducting pairing is expected to enhance rather than reduce the particle-hole symmetry.

Now we calculate the qp weight variationally with the Gutzwiller projected BCS-type wave functions. This kind of variational description is widely used in the study of the t-J model and is believed to capture the low energy physics of the cuprates[8, 9, 10, 11], especially when the doping is near optimal. The variational ground state, namely the Gutzwiller projected BCS state with N particle is given by(in the following we follow the notations of [5])

$$|\Psi_0^N\rangle = P_N P_G |\text{BCS}\rangle, \quad (1)$$

where P_N is projection onto the subspace of N particles, P_G is the projection onto the subspace of no double occupancy. $|\text{BCS}\rangle$ denotes the unprojected BCS mean field ground state. The elementary excitation above the ground state can be similarly constructed by Gutzwiller projection of BCS mean field excited state. For example, an particle-like elementary excitation is constructed as follows

$$|\Psi_{k,\sigma}^{N+1}\rangle = P_{N+1} P_G \gamma_{k,\sigma}^\dagger |\text{BCS}\rangle \quad (2)$$

where $\gamma_{k,\sigma}^\dagger$ is the creation operator for Bogliubov quasiparticle on the BCS mean field ground state which is related to the original electron operator $c_{k,\sigma}^\dagger$ through the Bogliubov transformation

$$\begin{pmatrix} \gamma_{k,\uparrow}^\dagger \\ \gamma_{-k,\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} u_{k^*} & -v_{k^*}^* \\ v_k & u_k \end{pmatrix} \begin{pmatrix} c_{k,\uparrow}^\dagger \\ c_{-k,\downarrow}^\dagger \end{pmatrix} \quad (3)$$

Similarly, a hole like elementary excitation with the same momentum and spin is constructed as follows

$$|\Psi_{k,\sigma}^{N-1}\rangle = P_{N-1} P_G \gamma_{k,\sigma}^\dagger |\text{BCS}\rangle \quad (4)$$

The qp weight for adding and removing an electron are given by the overlap between the corresponding bare electronic states and the qp states

$$Z_k^+ = \frac{|\langle \Psi_{k,\sigma}^{N+1} | c_{k,\sigma}^\dagger | \Psi_0^N \rangle|^2}{\langle \Psi_{k,\sigma}^{N+1} | \Psi_{k,\sigma}^{N+1} \rangle \langle \Psi_0^N | \Psi_0^N \rangle} \quad (5)$$

and

$$Z_k^- = \frac{|\langle \Psi_{k,\sigma}^{N-1} | c_{-k,-\sigma} | \Psi_0^N \rangle|^2}{\langle \Psi_{k,\sigma}^{N-1} | \Psi_{k,\sigma}^{N-1} \rangle \langle \Psi_0^N | \Psi_0^N \rangle} \quad (6)$$

As pointed out by Yunoki, using the fact that $P_G c_{k,\sigma}^\dagger P_G = P_G c_{k,\sigma}^\dagger [3]$, the qp weight for adding an electron can be related to the momentum distribution function n_k in the following way,

$$Z_k^+ = |u_k|^2 \frac{\langle \Psi_{k,\sigma}^{N+1} | \Psi_{k,\sigma}^{N+1} \rangle}{\langle \Psi_0^N | \Psi_0^N \rangle} = 1 - \frac{N_{\bar{\sigma}}}{L} - n_k \quad (7)$$

where $\frac{N_\sigma}{L}$ denotes the mean value of the particle number with opposite spin. Thus to calculate Z_k^+ , one only need to evaluate an ground state expectation value. The calculation of Z_k^+ is more complex. However, using $P_G c_{k,\sigma}^\dagger P_G = P_G c_{k,\sigma}^\dagger$ and the Bogliubov transformation Eq.(4), we are able to show that

$$Z_k^- = \alpha \frac{|u_k(v_k - u_k O_k)|^2}{Z_{k,N-2}^+} \quad (8)$$

where the constant α is given by

$$\alpha = \frac{\langle \Psi_0^N | \Psi_0^N \rangle}{\langle \Psi_0^{N-2} | \Psi_0^{N-2} \rangle} \quad (9)$$

and plays the role of the fugacity factor. O_k is given by following overlap integral

$$O_k = \frac{\langle \Psi_0^N | \Psi_{2k}^N \rangle}{\langle \Psi_0^N | \Psi_0^N \rangle} \quad (10)$$

in which

$$|\Psi_{2k}^N\rangle = P_N P_G \gamma_{k,\uparrow}^\dagger \gamma_{-k,\downarrow}^\dagger |\text{BCS}\rangle \quad (11)$$

Further simplification is possible when there is no superconducting pairing. In this case, one find

$$Z_k^+ = \frac{\langle \Psi_k^{N+1} | \Psi_k^{N+1} \rangle}{\langle \Psi_0^N | \Psi_0^N \rangle} \quad (12)$$

for k outside the Fermi surface and

$$Z_k^- = \frac{\langle \Psi_0^N | \Psi_0^N \rangle}{\langle \Psi_k^{N-1} | \Psi_k^{N-1} \rangle} \quad (13)$$

for k inside the Fermi surface. Noticing the fact that $|\Psi_k^{N+1}\rangle$ ($|\Psi_k^{N-1}\rangle$) is nothing but the variational ground state of the $N+1$ ($N-1$) system for k located on the Fermi surface, we have

$$Z_{k_F}^+ = \frac{\langle \Psi_0^{N+1} | \Psi_0^{N+1} \rangle}{\langle \Psi_0^N | \Psi_0^N \rangle} \quad (14)$$

$$Z_{k_F}^- = \frac{\langle \Psi_0^N | \Psi_0^N \rangle}{\langle \Psi_0^{N-1} | \Psi_0^{N-1} \rangle} \quad (15)$$

where k_F^\pm denotes momentum located on the Fermi surface. Thus, if the qp weight is a continuous function of particle number, it should be particle-hole symmetric in the thermodynamic limit. Furthermore, using Yunoki's relation and the fact that Z_k^+ vanish for k inside the Fermi surface, we have

$$n_k = 1 - \frac{n}{2} \quad (16)$$

for k inside the Fermi surface and

$$Z_{k_F}^+ = \Delta n_{k_F} \quad (17)$$

where Δn_{k_F} denotes the jump of n_k on the Fermi surface. Thus both Z_k^+ and Z_k^- converge to Δn_{k_F} on the Fermi surface in the thermodynamic limit, consistent with a Fermi liquid interpretation of the quasiparticle excitation.

We now present the result of VMC calculation. Fig.(1) shows the momentum distribution function and the qp weight for the Gutzwiller projected Fermi sea on a 18×18 lattice. Here the mean field Fermi sea is generated by a nearest neighboring hopping term on a square lattice with periodic-periodic boundary condition. The hole number is kept at 42 ($x \simeq 0.13$) so that the closed-shell condition is satisfied. As shown in Fig.1, the total qp weight is a continuous function of momentum across the Fermi surface. Thus the qp weight must be particle-hole symmetric on the Fermi surface in the thermodynamic limit, as we have argued before (note that the qp weight for adding (removing) an electron vanishes inside (outside) the Fermi surface). Note also that at this doping level the qp weight for removing an electron is only slightly higher than that for adding an electron in the whole Brillouin zone. Thus the quasiparticle contribution to the STM spectrum should be particle-hole symmetric at energy scale much smaller the band width.

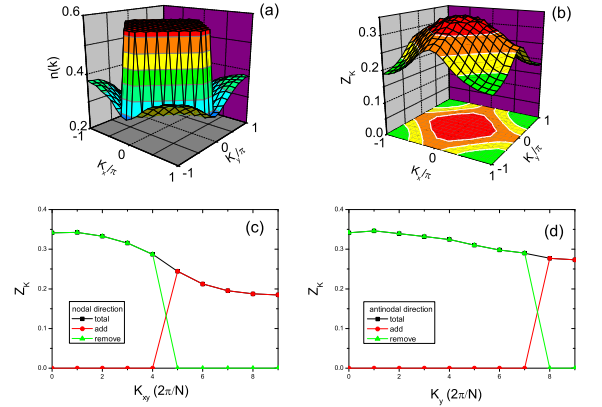


FIG. 1: VMC result for Gutzwiller projected Fermi sea on a 18×18 lattice with 42 holes ($x \simeq 0.13$). The hole density is chosen so that the closed shell condition is satisfied for system with periodic-periodic boundary condition. The mean field state is generated by nearest-neighbouring hopping term on the lattice. (a) momentum distribution function. (b) total qp weight. (c) qp weight in the $(0,0) - (\pi,\pi)$ direction. (d) qp weight in the $(0,0) - (0,\pi)$ direction.

Another implication of the above result is that most spectral weight in the hole side of the spectrum is incoherent. To show this more clearly, we plot in Fig.(2) the doping dependence of the $Z_{k=(0,0)}^-$ and $Z_{k=(\pi,\pi)}^+$. From the figure we see that both $Z_{k=(0,0)}^-$ and $Z_{k=(\pi,\pi)}^+$ van-

ish near half filling, in agreement with the slave-Boson mean field theory prediction. As compared to the slave-Boson mean field result($Z_k^+ = xu_k^2, Z_k^- = xv_k^2$), the qp weight calculated from projected wave function show more complex momentum dependence. The origin of the momentum dependence can be traced back to the non-monotonic behavior of $n(k)$. As first noted by in [12], the non-monotonic behavior of $n(k)$ comes from the correlated hopping nature of the electron in the t-J model. Another difference between the slave-Boson mean field theory and the projected wave function is the doping dependence of the qp weight(although they both vanish at half filling). In the slave-Boson mean field theory, the qp weight scales linearly with x at all momenta. However, we find the qp weight calculated from the projected wave function show x^{α_k} behavior at low doping, where α_k is a momentum dependent exponent. For the two dimensional projected Fermi sea, α_k increase monotonically from $\frac{1}{2}$ deep inside the Fermi surface to 1 far outside the Fermi surface. Thus the qp is more robust in the variational description than in the slave-Boson mean field theory. This difference may be caused by spin-charge recombination induced by the Gutzwiller projection[13].

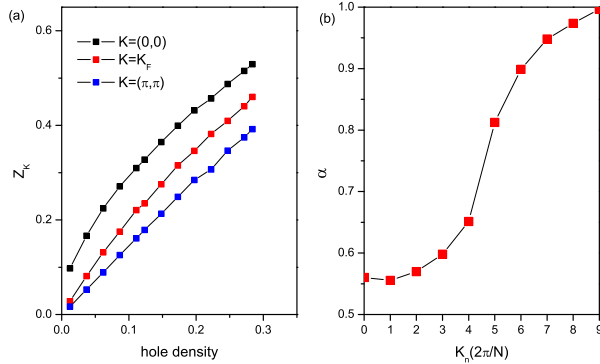


FIG. 2: Doping dependence of the qp weight as calculated from the Gutzwiller projected Fermi sea on a 18×18 lattice as a function of hole density. Periodic-antiperiodic boundary condition is used in the calculation to maximize the number of hole density that satisfy the closed-shell condition. (a) doping dependence of Z_k at three momenta along $(0, 0)$ to (π, π) , namely $k = (0, 0), k_F$ and (π, π) (note that since the boundary condition is periodic-antiperiodic, the momenta are not exactly in the nodal direction). (b) momentum dependence of the exponent α_k in the nodal direction.

Next we present the result for the Gutzwiller projected d-wave BCS state. The mean field state is generated by the following Hamiltonian

$$H_{MF} = - \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) - \mu \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma}$$

$$+ \Delta \sum_{\langle ij \rangle} d_{ij} (c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + c_{j\uparrow}^\dagger c_{i\downarrow}^\dagger + h.c.)$$

in which d_{ij} is the form factor for d-wave pairing and the sum is limited to nearest-neighboring sites. We take $\Delta = 0.1$ and the hole number is kept at 42. μ is determined by the mean field equation for density. Fig.(3) shows the momentum distribution function and the qp weight on a 18×18 lattice with periodic-periodic boundary condition. The result is basically the same as that of the projected Fermi sea state apart from the particle-hole mixture in the vicinity of the Fermi surface. One thing to note is that the total qp weight is a monotonic function of momentum in the nodal direction and do not exhibit pocket structure of the kind found for the Z_k^+ in [6]. To clarify the situation, we plot the momentum dependence of Z_k^+ and Z_k^- separately in Fig.(4). While a well defined pocket structure is observed in Z_k^+ , no corresponding structure exist in Z_k^- . The origin of the pocket structure in Z_k^+ can be traced back to the non-monotonic behavior of $n(k)$ around the nodal point as a result of the correlated hopping of electron in the t-J model and the d-wave pairing. However, Z_k^- do not show such pocket structure since it is a monotonically decreasing function of momentum in the nodal direction. At the same time, since the decrease of Z_k^+ in the $(0, \pi)$ to $(\pi, 0)$ direction due to pairing is compensated by the increase of Z_k^- , the total qp weight do not show pocket structure.

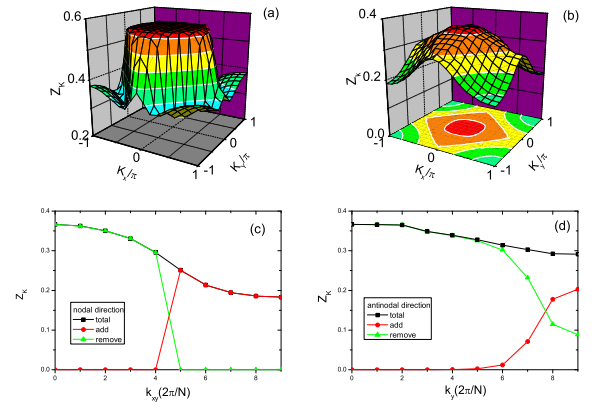


FIG. 3: VMC result for Gutzwiller projected d-wave BCS state on a 18×18 lattice with 42 holes ($x \simeq 0.13$) and $\frac{\Delta}{t} = 0.1$. (a) momentum distribution function. (b) total qp weight. (c) qp weight in the $(0, 0) - (\pi, \pi)$ direction. (d) qp weight in the $(0, 0) - (0, \pi)$ direction.

Above we have show that qp weight is particle-hole symmetric at sufficiently low energy. Thus the tunneling asymmetry at low energy should be attributed to the incoherent part of the electron spectrum. Since the electronic spectrum in the particle side is totally coherent, by

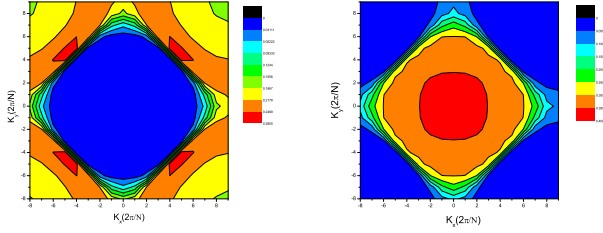


FIG. 4: Momentum dependence of Z_k^+ and Z_k^- in the Gutzwiller projected d-wave BCS state.

subtracting the STM spectrum on the hole side from that on the particle side we can extract the incoherent part of the electron spectrum. For strongly correlated system like cuprates, the information on the incoherent spectral weight is of great value. Through studying this spectrum, one can figure out the mechanism by which the bare electron decay into the many particle excitations and also the nature of the many particle excitations itself. In the context of the cuprates, two hotly discussed mechanisms to generate electron incoherence are scattering with some bosonic collective mode (like the neutron resonance mode)[14] and electron fractionalization as we have discussed in the slave-Boson mean field theory[2]. It is interesting to see which mechanism dominate the

tunneling asymmetry at low energy.

The author would like to thank members of the HTS group at CASTU for discussion. H.Y. Yang and T. Li is supported by NSFC Grant No. 90303009.

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